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Preprint 2015-23

Efficient algorithms for constraining orientation tensors in Galerkin methods for the Fokker-Planck equation

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Abstract

This paper deals with the problem of positivity preservation in numerical algorithms for simulating fiber suspension flows. In contrast to fiber orientation models based on the Advani-Tucker evolution equations for even-order orientation tensors, the probability distribution function of fiber orientation is approximated using the Galerkin discretization of the Fokker-Planck equation with Fourier basis functions or spherical harmonics. This procedure leads to a natural generalization of orientation tensor models replacing *ad hoc* closure approximations by Galerkin equations for the fine-scale components. After introducing an operator splitting approach to solving the discretized Fokker-Planck equation, we present conditions and correction techniques that guarantee physically correct distribution functions. As the reader will see, the derivation of these conditions is independent of the space dimension and their applicability is not limited to the simulation of fiber suspensions.

Keywords: fiber suspension flows, Fokker-Planck equation, orientation tensors, Galerkin approximation, Fourier analysis, spherical harmonics

1. Introduction

The simulation of complex two-phase flows is still one of the key challenges in the field of Computational Fluid Dynamics. While simple mixing processes only depend on the volume fractions of the two materials, the orientation of fibers transported by a fluid medium has a strong influence on the rheological behavior of fiber suspensions. If many fibers are aligned, the viscosity increases in the corresponding direction, and the mixture behaves

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more like a solid. Therefore, neglecting those effects may result in very inaccurate models that do not reproduce practical experiments very well.

In a typical fiber suspension model, the evolution equations introduced by Advani and Tucker [1] are used to calculate an orientation tensor of the distribution function. One disadvantage of this approach is the lack of a universal closure for higher-order tensors that appear in the evolution equations. Also, orientation tensors corresponding to distribution functions with negative values may arise. This could generate antidiffusive stress tensors in the Navier-Stokes equations and unphysical oscillations in the solution. In the worst case, the simulation may abort due to numerical instabilities.

Numerical solutions to the Fokker-Planck equation for the probability density function may also become negative leading to physically unrealistic predictions of local orientation states. While a variety of positivity-preserving schemes are available for simulating convective transport of scalar quantities in space and time, the presence of the divergence operator with respect to the orientation angles makes it more difficult to enforce positivity.

In this paper, we focus on the preservation of physical properties of orientation tensors. We prove that all even-order orientation tensors associated with a nonnegative probability density function are positive semi-definite. Then we derive and enforce sufficient conditions of positive semi-definiteness for a Galerkin discretization of the Fokker-Planck equation. The proposed correction techniques adjust the coefficients of Fourier basis functions or spherical harmonics so as to guarantee the physical correctness of orientation tensors in 2D/3D. The space-dependent part of the Fokker-Planck equation is decoupled using operator splitting. The corresponding subproblems and the Navier-Stokes equations for the velocity and pressure of the fiber suspension can be solved, e.g., using finite element schemes presented in [7, 11, 14]. For validation purposes, a numerical study is performed for planar flow problems with constant velocity gradients and known analytical solutions.

2. Fiber orientation modeling

Tracking the evolution of individual fibers is impossible and redundant when it comes to experimental and numerical studies of fiber suspension flows. The large number of fibers and immense costs associated with measurement or prediction of their properties call for a statistical approach to describing fiber orientation states. Therefore, we consider a (local) probability distribution function $\psi : \mathbb{R}^n \times \mathbb{S}^{n-1} \times \mathbb{R}_0^+ \to \mathbb{R}_0^+$ which specifies the probability $\psi(\mathbf{x}, \mathbf{p}, t)$ that a fiber occupying the space location $\mathbf{x} \in \mathbb{R}^n$ at the time instant $t \in \mathbb{R}_0^+$ has the orientation $\mathbf{p} \in \mathbb{S}^{n-1} \subset \mathbb{R}^n$. Based on this definition, ψ satisfies the normalization condition

$$\int_{\mathbb{S}^{n-1}} \psi(\mathbf{x}, \mathbf{p}, t)\, \mathrm{d}\mathbf{p} = 1 \qquad \text{for all } \mathbf{x} \in \mathbb{R}^n \text{ and } t \geq 0 \tag{1}$$

and possesses a positive parity due to the indistinguishability of the fiber ends

$$\psi(\cdot, \mathbf{p}, \cdot) = \psi(\cdot, -\mathbf{p}, \cdot) \qquad \text{for all orientations } \mathbf{p} \in \mathbb{S}^{n-1}. \tag{2}$$

The evolution of the probability distribution function ψ can be described by the (nonconservative form of the) Fokker-Planck equation [2, 8, 15]

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} + \nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}}\psi) = \frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi + \mathrm{div}_{\mathbf{p}}(\dot{\mathbf{p}}\psi) = D_r \Delta_{\mathbf{p}} \psi, \tag{3}$$

where $\mathbf{u}$ is the divergence-free velocity of the carrier fluid and $\dot{\mathbf{p}}$ is the time rate of change in the orientation $\mathbf{p}$ of a single fiber interacting with the fluid. This rotation rate can be modeled by the Jeffery equation [10]

$$\dot{\mathbf{p}} = \mathbf{W} \cdot \mathbf{p} + \lambda \left[\mathbf{D} \cdot \mathbf{p} - \mathbf{D} : (\mathbf{p} \otimes \mathbf{p})\mathbf{p} \right], \tag{4}$$

where $\mathbf{D} = \frac{1}{2}(\nabla_{\mathbf{x}}\mathbf{u} + \nabla_{\mathbf{x}}\mathbf{u}^\top)$ and $\mathbf{W} = \frac{1}{2}(\nabla_{\mathbf{x}}\mathbf{u} - \nabla_{\mathbf{x}}\mathbf{u}^\top)$ are the strain rate and vorticity tensors of the fluid and $\lambda = (r_e^2 - 1)(r_e^2 + 1)^{-1}$ is a parameter depending on the aspect ratio of the fibers $r_e = \frac{L}{d}$ with the fiber length L and the fiber diameter d. The right hand side of the Fokker-Planck equation (3) simulates possible fiber-fiber interactions using the Laplace-Beltrami operator $\Delta_{\mathbf{p}}$. Folgar and Tucker [9] define $D_r = C_I \dot{\gamma}$ with $\dot{\gamma} = (\frac{1}{2}\mathbf{D} : \mathbf{D})^{1/2}$ and an empirical constant $C_I \geq 0$ depending on the crowding number.

The Navier-Stokes equations for the velocity $\mathbf{u} \in \mathbb{R}^n$ and pressure $p \in \mathbb{R}_0^+$ of an incompressible mixture with density $\rho \in \mathbb{R}_0^+$ are given by

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \mathrm{div}_{\mathbf{x}}(\rho\mathbf{u} \otimes \mathbf{u}) = -\nabla_{\mathbf{x}} p + \mathrm{div}_{\mathbf{x}} \tau_{\text{eff}}, \qquad \mathrm{div}_{\mathbf{x}} \mathbf{u} = 0, \tag{5}$$

where τ_{eff} is the effective stress tensor of the mixture (see below).

Because of averaging processes $\mathbf{u}$ and ρ are defined by

$$\rho = (1 - \alpha)\rho_f + \alpha\rho_s, \tag{6a}$$

$$\rho\mathbf{u} = (1 - \alpha)\rho_f \mathbf{u}_f + \alpha\rho_s \mathbf{u}_s, \tag{6b}$$

where α is the volume fraction of fibers. The variables of the solid and fluid phase are denoted by ρ_s, $\mathbf{u}_s$ and ρ_f, $\mathbf{u}_f$, respectively. If we assume that the velocity of the fibers $\mathbf{u}_s$ is equal to the velocity of the mixture $\mathbf{u}$, we have

$$
\begin{aligned}
& (1-\alpha)\rho_f\mathbf{u}_f + \alpha\rho_s\mathbf{u}_s = \rho\mathbf{u} \\
\Leftrightarrow \quad & (1-\alpha)\rho_f\mathbf{u}_f + \alpha\rho_s\mathbf{u} \;= (1-\alpha)\rho_f\mathbf{u} + \alpha\rho_s\mathbf{u} \\
\Leftrightarrow \quad & (1-\alpha)\rho_f\mathbf{u}_f = (1-\alpha)\rho_f\mathbf{u}
\end{aligned}
\tag{7}
$$

and therefore $\mathbf{u} = \mathbf{u}_s = \mathbf{u}_f$.

This model for fiber suspensions is completed by the evolution equation for the volume fraction $\alpha : \mathbb{R}^n \times \mathbb{R}_0^+ \to [0,1]$

$$
\frac{\partial\alpha}{\partial t} + \mathrm{div}_{\mathbf{x}}(\mathbf{u}_s\alpha) = \frac{\partial\alpha}{\partial t} + \mathrm{div}_{\mathbf{x}}(\mathbf{u}\alpha) = 0 \tag{8}
$$

and a generic model for the effective stress tensor τ_{eff} [12]

$$
\begin{aligned}
\tau_{\text{eff}} &= 2\mu_{\text{eff}}\left[\mathbf{D} + N_p\mathbb{A}_4 : \mathbf{D} + N_s(\mathbb{A}_2\cdot\mathbf{D} + \mathbf{D}\cdot\mathbb{A}_2)\right], \\
\mu_{\text{eff}} &= \mu_0(1+\alpha H), \qquad N_p = \tfrac{\alpha E}{1+\alpha H}, \qquad N_s = \tfrac{\alpha B}{1+\alpha H},
\end{aligned}
\tag{9}
$$

where μ_0 is the dynamic viscosity of the fluid, H, E, B are positive material constants and $\mathbb{A}_2$ and $\mathbb{A}_4$ are the orientation tensors of second and fourth order, respectively, defined by $(1 \le i,j,k,l \le n)$

$$
\mathbb{A}_2 = (\mathbb{A}_{ij}), \qquad \mathbb{A}_{ij} = \langle \mathbf{p}_i\mathbf{p}_j\rangle = \int_{\mathbb{S}} \mathbf{p}_i\mathbf{p}_j\psi(\mathbf{p})\,\mathrm{d}\mathbf{p}, \tag{10a}
$$

$$
\mathbb{A}_4 = (\mathbb{A}_{ijkl}), \qquad \mathbb{A}_{ijkl} = \langle \mathbf{p}_i\mathbf{p}_j\mathbf{p}_k\mathbf{p}_l\rangle = \int_{\mathbb{S}} \mathbf{p}_i\mathbf{p}_j\mathbf{p}_k\mathbf{p}_l\psi(\mathbf{p})\,\mathrm{d}\mathbf{p}. \tag{10b}
$$

In a similar vein, an orientation tensor of order $m \in \mathbb{N}$ can be defined in terms of its components with $1 \le i_1, \ldots, i_m \le n$ as follows:

$$
\mathbb{A}_m = (\mathbb{A}_{i_1\ldots i_m}), \qquad \mathbb{A}_{i_1\ldots i_m} = \langle \mathbf{p}_{i_1}\ldots\mathbf{p}_{i_m}\rangle = \int_{\mathbb{S}} \mathbf{p}_{i_1}\ldots\mathbf{p}_{i_m}\psi(\mathbf{p})\,\mathrm{d}\mathbf{p}. \tag{10c}
$$

Notice that all orientation tensors $\mathbb{A}_m$ for odd m are equal to zero due to the positive parity of the orientation distribution function ψ.

The system of partial differential equations given by the Navier-Stokes equations (5) and the Fokker-Planck equation (3) models the macroscopic behavior of (semi-)dilute fiber suspension flows. As expected, there is a two-way coupling between (3) and (5) due to the dependence of the effective stress tensor τ_{eff} on the orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$ (and therefore on the orientation distribution function ψ) and the dependence of the rotation rate $\dot{\mathbf{p}}$ given by the Jeffery equation (4) on the spatial velocity gradient $\nabla_{\mathbf{x}}\mathbf{u}$.

If we multiply the Fokker-Planck equation (11) by the volume fraction α and add the evolution equation (8) multiplied by ψ, we obtain the following conservative formulation of the Fokker-Planck equation for the orientation probability density per unit volume $\tilde{\psi} = \alpha\psi$:

$$\begin{aligned} 0 &= \alpha\left(\frac{\partial\psi}{\partial t} + \mathbf{u}\cdot\nabla_{\mathbf{x}}\psi + \operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}}\psi) - D_r\Delta_{\mathbf{p}}\psi\right) + \psi\left(\frac{\partial\alpha}{\partial t} + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\alpha)\right) \\ &= \alpha\frac{\partial\psi}{\partial t} + \psi\frac{\partial\alpha}{\partial t} + \alpha\mathbf{u}\cdot\nabla_{\mathbf{x}}\psi + \psi\operatorname{div}_{\mathbf{x}}(\mathbf{u}\alpha) + \alpha\operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}}\psi) - \alpha D_r\Delta_{\mathbf{p}}\psi \\ &= \frac{\partial\alpha\psi}{\partial t} + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\alpha\psi) + \operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}}\alpha\psi) - D_r\Delta_{\mathbf{p}}(\alpha\psi) \\ &= \frac{\partial\tilde{\psi}}{\partial t} + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\tilde{\psi}) + \operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}}\tilde{\psi}) - D_r\Delta_{\mathbf{p}}\tilde{\psi}. \end{aligned} \tag{11}$$

By definition, $\tilde{\psi}(\mathbf{x},\mathbf{p},t)$ describes the probability of discovering a fiber with an orientation $\mathbf{p}$ at the space location $\mathbf{x}$ and time t. By (1) we have

$$\alpha(\mathbf{x},t) = \oint_{\mathbb{S}^{n-1}} \tilde{\psi}(\mathbf{x},\mathbf{p},t)\,\mathrm{d}\mathbf{p} \qquad \text{for all } x\in\mathbb{R}^n \text{ and } t\geq 0. \tag{12}$$

In the following, we will always use the α-weighted form of the orientation distribution and omit the tilde $\tilde{\cdot}$ for brevity. In particular, the orientation tensors $\mathbb{A}_m$ are defined by the volumetric probability density $\tilde{\psi}$. If we consider the space-independent formulation of the Fokker-Planck equation (11), the two definitions of the orientation distribution function are equivalent.

3. Galerkin discretization

In this section, we focus on the discretization of the Fokker-Planck equation (11). Multiplying it by $\mathbf{p}_i\mathbf{p}_j$, integrating over the sphere $\mathbb{S}^{n-1}$ and invoking the definition of the orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$, one obtains the evolution equation introduced by Advani and Tucker [1]

$$\frac{\mathrm{d}\mathbb{A}_2}{\mathrm{d}t} = (\mathbf{W}\mathbb{A}_2 - \mathbb{A}_2\mathbf{W}) + \lambda(\mathbf{D}\mathbb{A}_2 + \mathbb{A}_2\mathbf{D} - 2\mathbb{A}_4 : \mathbf{D}) + 2D_r(\boldsymbol{\mathcal{I}} - n\mathbb{A}_2). \tag{13}$$

This popular fiber orientation model represents a second-order moment approximation to the Fokker-Planck equation.

Similarly, evolution equations for orientation tensors $\mathbb{A}_m$ of higher order $m = 2k,\ k > 1$ can be derived by multiplying the Fokker-Planck equation (11) by $\mathbf{p}_{i_1} \dots \mathbf{p}_{i_m}$ and integrating over the sphere $\mathbb{S}^{n-1}$. A common drawback of such moment approximations is the necessity of an empirical closure for the orientation tensor of the next higher order $\mathbb{A}_{m+2} \approx \tilde{\mathbb{A}}_{m+2}(\mathbb{A}_m)$ to obtain a closed formulation (such as equation (13) with the unknown tensor $\mathbb{A}_4$ approximated by a function of $\mathbb{A}_2$). There are many closure approximations based on different modeling approaches like the linear, quadratic, and hybrid closure from the paper by Advani and Tucker [1] and orthotropic closures derived by Cintra and Tucker [6]. Unfortunately, none of these closures is able to model the tensor $\mathbb{A}_4$ correctly in all possible test cases.

Here we introduce another, more general approach to deriving a discrete version of the Fokker-Planck equation (11) based on an operator splitting approach to time integration, Galerkin discretizations of the corresponding PDEs, and a customized tensor product ansatz to avoid the use of closure approximations and minimize the dimension of the subproblems.

To decompose the Fokker-Planck equation (11) into subproblems with segregated treatment of the convective transport in space and orientation changes at a fixed location, we define the differential operators $\mathcal{L}_{\mathbf{x}}$ and $\mathcal{L}_{\mathbf{p}}$ w.r.t. the space and orientation variables, respectively, as follows:

$$\mathcal{L}_{\mathbf{x}} \cdot = \operatorname{div}_{\mathbf{x}}(\mathbf{u} \cdot), \tag{14a}$$

$$\mathcal{L}_{\mathbf{p}} \cdot = \operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}} \cdot) - D_r \Delta_{\mathbf{p}} \cdot . \tag{14b}$$

This decomposition of $\mathcal{L} = \mathcal{L}_{\mathbf{x}} + \mathcal{L}_{\mathbf{p}}$ makes it possible to discretize the Fokker-Planck equation (11) in time using an operator splitting approach. In the simplest case, we have to solve the following initial value problems:

$$\frac{\partial \psi^{(\mathbf{p})}}{\partial t} + \mathcal{L}_{\mathbf{p}} \psi^{(\mathbf{p})} = 0 \qquad \text{for } t \in (t^n, t^{n+1}) \qquad \text{with} \qquad \psi^{(\mathbf{p})}(t^n) = \psi^n, \tag{15a}$$

$$\frac{\partial \psi^{(\mathbf{x})}}{\partial t} + \mathcal{L}_{\mathbf{x}} \psi^{(\mathbf{x})} = 0 \qquad \text{for } t \in (t^n, t^{n+1}) \qquad \text{with} \qquad \psi^{(\mathbf{x})}(t^n) = \psi^{(\mathbf{p})}(t^{n+1}) \tag{15b}$$

for discrete time levels $t^0 = 0 < t^1 < \ldots < t^M = T$ with the initial condition $\psi^0 = \psi_0$. The final orientation distribution $\psi^{(\mathbf{x})}(t^{n+1})$ approximates the solution of the Fokker-Planck equation (11) at the time level t^{n+1}, that is, $\psi^{n+1} = \psi^{(\mathbf{x})}(t^{n+1}) \approx \psi(t^{n+1})$. Further discretization of the two subproblems is based on the tensor product ansatz

$$\psi(\mathbf{x},\mathbf{p},t)=\sum_{i,j}\psi_{i,j}(t)\sigma_i(\mathbf{x})\varrho_j(\mathbf{p}) \quad \in \quad V=\operatorname{span}\{\sigma_i\varrho_j\} \tag{16}$$

with a currently arbitrary orthonormal basis $\{\varrho_j\}$ in the orientation direction and linear finite elements $\{\sigma_i\}$ in the space direction for the orientation distribution function ψ. Using $\sigma_k\varrho_l$ as test functions in the weak formulation and substituting (16), one obtains the semi-discrete problems

$$\begin{aligned}0=\int_\Omega\oint_{\mathbb{S}}\sigma_k(\mathbf{x})\varrho_l(\mathbf{p})\sum_{i,j}\sigma_i(\mathbf{x})\Big[\dot{\psi}_{i,j}(t)\varrho_j(\mathbf{p})+\psi_{i,j}(t)\big(\operatorname{div}_{\mathbf{p}}(\dot{\mathbf{p}}\varrho_j(\mathbf{p}))\\ -D_r\Delta_{\mathbf{p}}\varrho_j(\mathbf{p})\Big]\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{x},\end{aligned} \tag{17a}$$

$$0=\int_\Omega\oint_{\mathbb{S}}\sigma_k(\mathbf{x})\varrho_l(\mathbf{p})\sum_{i,j}\varrho_j(\mathbf{p})\left[\dot{\psi}_{i,j}(t)\sigma_i(\mathbf{x})+\psi_{i,j}(t)\operatorname{div}_{\mathbf{x}}(\mathbf{u}\sigma_i(\mathbf{x}))\right]\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{x} \tag{17b}$$

for all k,l. After performing mass lumping in equation (17a) and exploiting the orthonormality of the basis functions σ_i in equation (17b), these equations yield the semi-discrete versions of the space- and orientation-independent Fokker-Planck equation (11)

$$\frac{\partial\psi(\mathbf{p},t)}{\partial t}+\operatorname{div}_{\mathbf{p}}\left(\dot{\mathbf{p}}\psi(\mathbf{p},t)\right)-D_r\Delta_{\mathbf{p}}\psi(\mathbf{p},t)=0, \tag{18}$$

$$\frac{\partial\psi(\mathbf{x},t)}{\partial t}+\operatorname{div}_{\mathbf{x}}\left(\mathbf{u}\psi(\mathbf{x},t)\right)=0, \tag{19}$$

respectively. When it comes to calculating $\dot{\mathbf{p}}$ in equation (18), the velocity gradient $\nabla_{\mathbf{x}}\mathbf{u}$ is evaluated at the grid node associated with the basis function σ_i. Equation (19) represents an ordinary spatial convection problem with the velocity $\mathbf{u}$ and no diffusion. Numerical methods for solving such equations are already extensively discussed in the literature (see, e.g., [7, 11, 14] and references therein). For this reason, we will disregard (19) in the next sections but keep in mind that a spatial convection step of this form must be performed for each degree of freedom of the orientation discretization. On the other hand, we must solve the space-independent Fokker-Planck equation (18) at each node of the spatial grid. So it is beneficial to reduce the number of degrees of freedom in the orientation discretization and minimize the computational effort for simulating orientation changes. Therefore, the key challenge of the next sections will be the development of a new approach to constructing good physics-compatible approximations of the space-independent orientation distribution function ψ with a small number of degrees of freedom.

4. Fourier analysis in 2D

As already mentioned, a physically meaningful distribution function $\psi(\mathbf{p})$ should be nonnegative for all possible orientations $\mathbf{p} \in \mathbb{S}^{n-1}$. Otherwise, the corresponding orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$ and therefore the effective stress tensor τ_{eff} defined by equation (9) could be physics-incompatible. To preserve the nonnegativity property at the discrete level, we could use locally defined interpolatory basis functions like linear finite elements and impose positivity constraints on the nodal values of the numerical solution. However, a relatively large number of degrees of freedom would be needed to approximate the distribution function ψ and to compute the corresponding orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$ for the effective stress tensor τ_{eff} accurately enough. Moreover, it would be expensive to enforce the normalization condition (1) or (12).

In this paper, we favor globally defined trigonometric basis functions which simplify the preservation of mass and possess the orthonormality property, as required by the operator splitting algorithm described in the last section. More specifically, we choose the normalized Fourier basis functions

$$\varrho_j(\phi) = \begin{cases} \frac{1}{\sqrt{2\pi}} & : j = 0, \\ \frac{1}{\sqrt{\pi}} \sin\left((j+1)\phi\right) & : j \text{ is odd}, \\ \frac{1}{\sqrt{\pi}} \cos\left(j\phi\right) & : j \text{ is even} \end{cases} \tag{20}$$

in the case of planar orientation distribution functions $\psi : \mathbb{S}^1 \subset \mathbb{R}^2 \to \mathbb{R}_0^+$. The case of a three-dimensional orientation distribution is treated in section 6.

If ψ is square integrable and has a positive parity, then it can be represented by a Fourier expansion in polar coordinates $\mathbf{p}(\phi) = (\cos\phi, \sin\phi)^\top$

with $\phi \in [0, 2\pi)$. We have

$$\begin{aligned}\psi(\phi) &= a_0 \tfrac{1}{\sqrt{2\pi}} + \tfrac{1}{\sqrt{\pi}} \sum_{j\in\mathbb{N}} \left(a_{2j}\cos(2j\phi) + b_{2j}\sin(2j\phi)\right) \\ &= a_0\varrho_0(\phi) + \sum_{j\in\mathbb{N}} \left(a_{2j}\varrho_{2j}(\phi) + b_{2j}\varrho_{2j-1}(\phi)\right) = \sum_{j\in\mathbb{N}_0} \psi_j \varrho_j(\phi)\end{aligned} \tag{21}$$

with the Fourier coefficients $a_0, a_j, b_j \in \mathbb{R}$, $j \in 2\mathbb{N}$, or $\psi_j \in \mathbb{R}$, $j \in \mathbb{N}_0$, and $\psi_{2j} = a_{2j}$ and $\psi_{2j+1} = b_{2j+2}$, $j \in \mathbb{N}_0$, defined by

$$a_{2i} = \int_0^{2\pi} \psi(\phi)\cos(2i\phi)\,\mathrm{d}\phi = \int_0^{2\pi} \psi(\phi)\varrho_{2i}(\phi)\,\mathrm{d}\phi \qquad i \in \mathbb{N}_0, \tag{22a}$$

$$b_{2i} = \int_0^{2\pi} \psi(\phi)\sin(2i\phi)\,\mathrm{d}\phi = \int_0^{2\pi} \psi(\phi)\varrho_{2i+1}(\phi)\,\mathrm{d}\phi \qquad i \in \mathbb{N}_0. \tag{22b}$$

So the obvious discretization procedure is to use a truncated Fourier series of order $N_\mathbf{p} \in 2\mathbb{N}$ as an approximation for ψ

$$\psi^{N_\mathbf{p}}(\phi) = \psi \sum_{j=0}^{N_\mathbf{p}} \psi_j \varrho_j(\phi) \quad \approx \quad \psi(\phi) \tag{23}$$

and test the weak formulation of the space-independent Fokker-Planck equation (18) with the basis functions ϱ_i, $0 \le i \le N_\mathbf{p}$.

One advantage of this approach is the trivial and natural implementation of the normalization condition (1) or (12): the "mass" of ψ is only depending on the first Fourier coefficient $\psi_0 = a_0$

$$\int_0^{2\pi} \psi^{N_\mathbf{p}}(\phi)\,\mathrm{d}\phi = \sqrt{2\pi} \sum_{j=0}^{N_\mathbf{p}} \psi_j \int_0^{2\pi} \varrho_j(\phi)\varrho_0(\phi)\,\mathrm{d}\mathbf{p} = \sqrt{2\pi}a_0. \tag{24}$$

On the other hand, it is not clear what $\psi^{N_\mathbf{p}} \ge 0$ means for a Fourier approximation of a finite order $N_\mathbf{p} \in 2\mathbb{N}$:

If we require that $\psi^{N_\mathbf{p}}(\phi)$ be nonnegative for all possible orientations $\phi \in [0, 2\pi)$, then the exact truncated Fourier series $\mathcal{P}_{N_\mathbf{p}}\psi$ of a nonnegative orientation distribution function ψ may not be acceptable (see Figure 1). In addition, it is very expensive to find the minimum of $\psi^{N_\mathbf{p}}$ for orders $N_\mathbf{p} > 2$ due to the global definition of the basis functions ϱ_j.

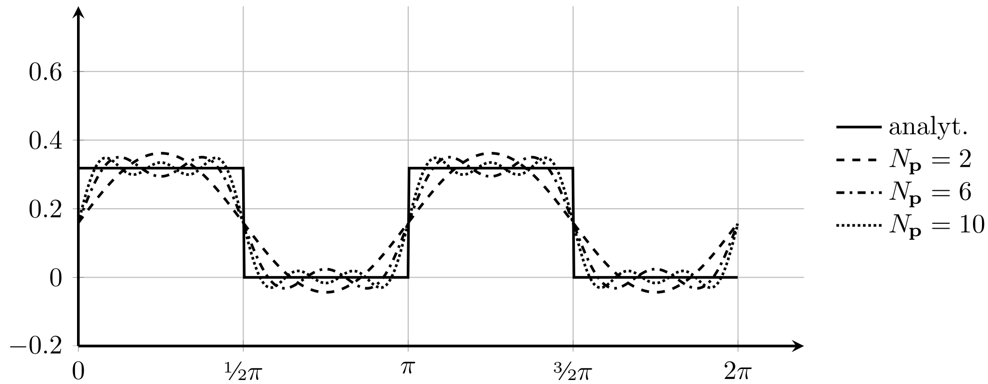

Figure 1: Demonstration of the Gibbs phenomenon for different orders $N_{\mathbf{p}}$.

Another possible interpretation of the nonnegativity condition is the following: There exists a function $\bar{\psi} \geq 0$ with $\mathcal{P}_{N_{\mathbf{p}}} \bar{\psi} = \psi^{N_{\mathbf{p}}}$, which is the same as the equality of the first Fourier coefficients, $\bar{\psi}_j = \psi_j$ for all $0 \leq j \leq N_{\mathbf{p}}$. This is a more realistic choice for the condition $\psi^{N_{\mathbf{p}}} \geq 0$, because the truncated Fourier series $\mathcal{P}_{N_{\mathbf{p}}} \psi$ is accepted for every $\psi \geq 0$ no matter if $\psi^{N_{\mathbf{p}}}(\phi) \geq 0$ holds for all $\phi \in [0, 2\pi)$ or not. The disadvantage is that the function $\psi \geq 0$ with $\mathcal{P}_{N_{\mathbf{p}}} \psi = \psi^{N_{\mathbf{p}}}$ is generally unknown and therefore we may not know if our approximation fulfills this interpretation of the condition $\psi^{N_{\mathbf{p}}} \geq 0$. Nevertheless, it is possible to derive necessary constraints for the Fourier coefficients of a nonnegative function $\psi \geq 0$. For example, we have

$$\begin{aligned} |a_{2i}| &= \frac{1}{\sqrt{\pi}} \Big| \int_0^{2\pi} \psi(\phi) \cos(2i\phi) \,\mathrm{d}\phi \Big| \leq \frac{1}{\sqrt{\pi}} \int_0^{2\pi} \psi(\phi) \left|\cos(2i\phi)\right| \,\mathrm{d}\phi \\ &\leq \frac{1}{\sqrt{\pi}} \int_0^{2\pi} \psi(\phi) \,\mathrm{d}\phi \leq \sqrt{2} \int_0^{2\pi} \psi(\phi) \varrho_0(\phi) \,\mathrm{d}\phi = \sqrt{2} a_0 \end{aligned} \tag{25a}$$

$$|b_{2i}| = \frac{1}{\sqrt{\pi}} \Big| \int_0^{2\pi} \psi(\phi) \sin(2i\phi) \,\mathrm{d}\phi \Big| \leq \sqrt{2} a_0, \tag{25b}$$

or, more generally,

$$c_{2i} = \Big| \frac{1}{\sqrt{\pi}} \int_0^{2\pi} \psi(\phi) \cos(2i\phi + \kappa) \,\mathrm{d}\phi \Big| \leq \sqrt{2} a_0 \tag{25c}$$

with $c_{2i} = \sqrt{a_{2i}^2 + b_{2i}^2}$ and $\kappa \in [0, \frac{\pi}{i})$ defined by

$$b_{2i} \cos(2i\phi) + a_{2i} \sin(2i\phi) = c_k \cos(2i\phi + \kappa). \tag{26}$$

In this section, we will develop a new approach to constructing additional inequality constraints depending on (orientation) tensors more general than those defined in equations (10). For this purpose, we use the property of positive semi-definiteness of the tensors and focus on the coefficients of the characteristic polynomial.

Before analyzing the orientation tensors, we start with a useful interpretation of an arbitrary tensor. Each tensor $\mathbb{B} \in \mathbb{R}^{n\times\ldots\times n}$ of an arbitrary order $2m \in \mathbb{N}$ (this means $n \times \ldots \times n$ $2m$ times) can be interpreted as a matrix $\mathbf{B} \in \mathbb{R}^{n^m \times n^m}$. The equivalence relation is given by the transformation $\varsigma : \{1, \ldots, n\}^m \to \{1, \ldots, n^m\}$ defined by

$$\varsigma(i_1, \ldots, i_m) = \sum_{k=1}^{m} n^{k-1}(i_k - 1)^m + 1. \tag{27}$$

Then the components of $\mathbf{B}$ are uniquely defined by

$$\mathbf{B}_{\varsigma(i_1,\ldots,i_m),\varsigma(i_{m+1},\ldots,i_{2m})} = \mathbb{B}_{i_1\ldots i_{2m}}. \tag{28}$$

This relation motivates the following definition of positive definiteness of a general tensor, which is a generalization of a definition by Vincenzi [16].

Defintion 4.1 (Positive definiteness of a tensor)**.** *A tensor* $\mathbb{B} \in \mathbb{R}^{n\times\ldots\times n}$*,* $n \in \mathbb{N}$ *of order* $2m \in 2\mathbb{N}$ *(i.e.,* $n \times \ldots \times n$ $2m$ *times) is positive definite if and only if*

$$\mathbf{S}_{i_1\ldots i_m}\mathbb{B}_{i_1\ldots i_m j_1\ldots j_m}\mathbf{S}_{j_1\ldots j_m} = \mathbf{S} : (\mathbb{B} : \mathbf{S}) > 0 \qquad \textit{for all } \mathbf{S} \in \mathbb{R}^{n\times\ldots\times n}\backslash\{\mathbf{0}\}, \tag{29}$$

where $\mathbf{S} \in \mathbb{R}^{n\times\ldots\times n}$ *is a tensor of order* m*.*

Other properties like the positive semi-definiteness are defined in a similar way. This enables us to formulate and prove the following theorem.

Theorem 4.1 (Positive semi-definiteness of an orientation tensor)**.** *Let* $\psi \geq 0$ *be a nonnegative function. Then each orientation tensor* $\mathbb{A}_{2m}$ *of order* $2m \in 2\mathbb{N}$ *defined by equation* (10) *is positive semi-definite.*

Proof. For each tensor $\mathbf{S} \in \mathbb{R}^{n\times\ldots\times n}$ of order m we have

$$
\begin{aligned}
&\sum_{1\le i_1\ldots i_m j_1\ldots j_m\le n} \mathbf{S}_{i_1\ldots i_m}\mathbb{A}_{i_1\ldots i_m j_1\ldots j_m}\mathbf{S}_{j_1\ldots j_m} \\
&= \sum_{1\le i_1\ldots i_m\le n} \mathbb{A}_{i_1\ldots i_m i_1\ldots i_m}\mathbf{S}^2_{i_1\ldots i_m} + 2\sum_{\substack{1\le i_1\ldots i_m j_1\ldots j_m\le n,\\ (i_1\ldots i_m)<(j_1\ldots j_m)}} \mathbb{A}_{i_1\ldots i_m j_1\ldots j_m}\mathbf{S}_{i_1\ldots i_m}\mathbf{S}_{j_1\ldots j_m} \\
&= \int_{\mathbb{S}^{n-1}} \psi(\mathbf{p}) \sum_{1\le i_1\ldots i_m\le n} (\mathbf{p}_{i_1}\ldots\mathbf{p}_{i_m})^2\mathbf{S}^2_{i_1\ldots i_m}\,\mathrm{d}\mathbf{p} \\
&\quad + 2\int_{\mathbb{S}^{n-1}} \psi(\mathbf{p}) \sum_{\substack{1\le i_1\ldots i_m j_1\ldots j_m\le n,\\ (i_1\ldots i_m)<(j_1\ldots j_m)}} \mathbf{p}_{i_1}\ldots\mathbf{p}_{i_m}\mathbf{p}_{j_1}\ldots\mathbf{p}_{j_m}\mathbf{S}_{i_1\ldots i_m}\mathbf{S}_{j_1\ldots j_m}\mathrm{d}\mathbf{p} \\
&= \int_{\mathbb{S}^{n-1}} \psi(\mathbf{p})\Big(\sum_{1\le i_1\ldots i_m\le n} \mathbf{p}_{i_1}\ldots\mathbf{p}_{i_m}\mathbf{S}_{i_1\ldots i_m}\Big)^2\mathrm{d}\mathbf{p} \ge 0
\end{aligned}
$$

because of $\psi \ge 0$. This proves the assertion. □

This result makes it possible to derive conditions for the Fourier coefficients by analyzing the eigenvalues of the orientation tensors. For example, a general procedure would be the calculation of $\mathbb{A}_2$ by definition (10a) and checking the signs of the corresponding eigenvalues. If negative eigenvalues are found, the Fourier coefficients have to be corrected to satisfy the requirement of positive semi-definiteness. It is also possible to express the orientation tensors in terms of the Fourier coefficients. Then there is no need to calculate the integrals of definition (10) in each correction step. In addition, inequalities for the Fourier coefficients can be derived a priori using the corresponding characteristic polynomials and Descartes' rule of signs [3, 5].

Theorem 4.2 (Descartes' rule of signs)**.** *Let $p(x) = p_n x^n + p_{n-1}x^{n-1} + \ldots + p_0$ be a polynomial with real coefficients $p_0, \ldots, p_n \in \mathbb{R}$, s be the number of sign changes between consecutive nonzero coefficients of the sequence $(p_n, \ldots, p_0)$ and t be the number of positive roots of the polynomial p .Then the difference $s - t$ is a nonnegative even integer.*

A variation of sign in the sequence $(p_n, \ldots, p_0)$ occurs if and only if $p_i p_j < 0$ for $j = i + 1$ or $j > i + 1$ with $p_k = 0$ for all $i < k < j$.

Applying theorem 4.2 to the polynomial

$$\tilde{p}(x) = p(-x) = (-1)^n p_n x^n + (-1)^{n-1} p_{n-1} x^{n-1} + \ldots + p_0, \tag{30}$$

we find that p has no negative root ($\tilde{p}$ has no positive root) if and only if $(-1)^k p_k \geq 0$ or $(-1)^k p_k \leq 0$ for all $0 \leq k \leq n$. The direction that does not follow from theorem 4.2 could be proven trivially by expanding

$$p(x) = (x - \alpha_1) \cdot \ldots \cdot (x - \alpha_n), \tag{31}$$

where $\alpha_1, \ldots, \alpha_n \geq 0$ are the nonnegative roots of the polynomial.

Using this result, we can prove the core statement of this paper which is applicable to an arbitrary orientation tensor $\mathbb{A}_{2m}$.

Theorem 4.3 (Positive semi-definiteness of a tensor)**.** *A symmetric tensor $\mathbb{B} \in \mathbb{R}^{n \times \ldots \times n}$ of order $2m \in 2\mathbb{N}$ is positive semi-definite if and only if the characteristic polynomial*

$$\chi_{\mathbb{B}}(\lambda) := \chi_{\mathbf{B}}(\lambda) = \det(\lambda \boldsymbol{\mathcal{I}} - \mathbf{B}) = \lambda^{n^m} + p_{n^m-1}\lambda^{n^m-1} + \ldots + p_0 \tag{32}$$

of the corresponding matrix $\mathbf{B} \in \mathbb{R}^{n^m \times n^m}$ defined by equation (28) *fulfills the condition*

$$(-1)^{n^m - k} p_k \geq 0 \qquad \textit{for all } 0 \leq k < n^m. \tag{33}$$

Proof. First we note that all eigenvalues of $\mathbf{B}$ and therefore $\mathbb{B}$ are real-valued due to the symmetry of $\mathbb{B}$. Additionally, inequalities (33) ensure that there is no negative root of $\chi_{\mathbb{B}}$ and therefore no negative eigenvalue of $\mathbb{B}$, which completes the proof. $\square$

To derive conditions for the first Fourier coefficients of our approximation $\psi^{N_{\mathbf{P}}}$ making use of theorem 4.3, let us define a generalization of the second order orientation tensor $\mathbb{B}_2^{(m)} \in \mathbb{R}^{2\times 2}$, $m \in 2\mathbb{N}$ thus:

$$\begin{aligned}
\mathbb{B}_2^{(m)} &= \int_0^{2\pi} \begin{pmatrix} \cos(\frac{m}{2}\phi)\cos(\frac{m}{2}\phi) & \cos(\frac{m}{2}\phi)\sin(\frac{m}{2}\phi) \\ \sin(\frac{m}{2}\phi)\cos(\frac{m}{2}\phi) & \sin(\frac{m}{2}\phi)\sin(\frac{m}{2}\phi) \end{pmatrix} \psi(\phi)\,\mathrm{d}\phi \\
&= \frac{1}{2}\int_0^{2\pi} \begin{pmatrix} 1 + \cos(m\phi) & \sin(m\phi) \\ \sin(m\phi) & 1 - \cos(m\phi) \end{pmatrix} \psi(\phi)\,\mathrm{d}\phi \\
&= \frac{\sqrt{\pi}}{2}\int_0^{2\pi} \begin{pmatrix} \sqrt{2}\varrho_0 + \varrho_m & \varrho_{m-1} \\ \varrho_{m-1} & \sqrt{2}\varrho_0 - \varrho_m \end{pmatrix} \psi(\phi)\,\mathrm{d}\phi \\
&= \frac{\sqrt{\pi}}{2} \begin{pmatrix} \sqrt{2}a_0 + a_m & b_m \\ b_m & \sqrt{2}a_0 - a_m \end{pmatrix}.
\end{aligned} \tag{34}$$

Notice that $\mathbb{B}_2^{(2)}$ is equal to $\mathbb{A}_2$. The characteristic polynomial of such a tensor is given by

$$\begin{aligned}
\chi_{\mathbb{B}_2^{(m)}}(\lambda) &= \det(\lambda \boldsymbol{\mathcal{I}} - \mathbb{B}_2^{(m)}) = \det(\tfrac{\sqrt{\pi}}{2}\tilde{\lambda}\boldsymbol{\mathcal{I}} - \mathbb{B}_2^{(m)}) \\
&= \frac{\pi}{4}\left(\left(\tilde{\lambda} - \sqrt{2}a_0 - a_m\right)\left(\tilde{\lambda} - \sqrt{2}a_0 + a_m\right) - b_m^2\right) \\
&= \frac{\pi}{4}\left(\tilde{\lambda}^2 - 2\sqrt{2}a_0\tilde{\lambda} + 2a_0^2 - a_m^2 - b_m^2\right),
\end{aligned} \tag{35}$$

where $\tilde{\lambda} = \frac{2\lambda}{\sqrt{\pi}}$. This yields the inequalities

$$\begin{cases} 0 \le a_0, & \text{(36a)} \\ 0 \le 2a_0^2 - a_m^2 - b_m^2 = 2a_0^2 - c_m^2 & \text{(36b)} \end{cases}$$

because of the positive semi-definiteness of $\mathbb{B}_2^{(m)}$. Condition (36a) is trivially satisfied due to the normalization condition (12) and inequality (36b) is equivalent to equation (25c). Thus we have derived the inequality constraint $2a_0^2 \ge a_k^2 + b_k^2$ for the Fourier coefficients a_k and b_k in another way.

Next we analyze the fourth order orientation tensor $\mathbb{A}_4$. Using the addition theorems for trigonometric polynomials and the orthonormality of the basis functions ϱ_j, the fourth order orientation tensor can be written as

$$\mathbb{A}_4 = \tfrac{\sqrt{\pi}}{8}\begin{pmatrix} 3\sqrt{2}a_0 + 4a_2 + a_4 & 2b_2 + b_4 & 2b_2 + b_4 & \sqrt{2}a_0 - a_4 \\ 2b_2 + b_4 & \sqrt{2}a_0 - a_4 & \sqrt{2}a_0 - a_4 & 2b_2 - b_4 \\ 2b_2 + b_4 & \sqrt{2}a_0 - a_4 & \sqrt{2}a_0 - a_4 & 2b_2 - b_4 \\ \sqrt{2}a_0 - a_4 & 2b_2 - b_4 & 2b_2 - b_4 & 3\sqrt{2}a_0 - 4a_2 + a_4 \end{pmatrix}. \tag{37}$$

Let $\lambda \in \mathbb{R}$ and $\tilde{\lambda} = \frac{\lambda}{\sqrt{\pi}}$. The characteristic polynomial of $\mathbb{A}_4$ is given by

$$\begin{aligned}
\chi_{\mathbb{A}_4}(\lambda) &= \det(\lambda \boldsymbol{\mathcal{I}} - \mathbb{A}_4) = \det(\sqrt{\pi}\tilde{\lambda}\boldsymbol{\mathcal{I}} - \mathbb{A}_4) \\
&= -\tfrac{\pi^2}{32}\tilde{\lambda}\Big(2\sqrt{2}a_0^3 - 20a_0^2\tilde{\lambda} - 2\sqrt{2}a_0a_2^2 - \sqrt{2}a_0a_4^2 - 2\sqrt{2}a_0b_2^2 - \sqrt{2}a_0b_4^2 \\
&\qquad + 32\sqrt{2}a_0\tilde{\lambda}^2 + 2a_2^2a_4 + 8a_2^2\tilde{\lambda} + 4a_2b_2b_4 + 2a_4^2\tilde{\lambda} - 2a_4b_2^2 \\
&\qquad + 8b_2^2\tilde{\lambda} + 2b_4^2\tilde{\lambda} - 32\tilde{\lambda}^3\Big) \\
&= -\tfrac{\pi^2}{32}\tilde{\lambda}\Big(-32\tilde{\lambda}^3 + 32\sqrt{2}a_0\tilde{\lambda}^2 - (20a_0^2 - 8c_2^2 - 2c_4^2)\tilde{\lambda} \\
&\qquad + 2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2\Big) \\
&= \pi^2\tilde{\lambda}^4 - \pi^2\sqrt{2}a_0\tilde{\lambda}^3 + \tfrac{\pi^2}{16}(10a_0^2 - 4c_2^2 - c_4^2)\tilde{\lambda}^2 \\
&\quad - \tfrac{\pi^2}{32}(2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2).
\end{aligned}$$

This reveals the following conditions

$$\begin{cases}
0 \le a_0, & \text{(38a)} \\
0 \le 10a_0^2 - 4c_2^2 - c_4^2, & \text{(38b)} \\
0 \le 2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2, & \text{(38c)}
\end{cases}$$

where inequality (38a) is again satisfied by the normalization condition (12) and inequality (38b) is satisfied by condition (25c) for $i = 1, 2$

$$10a_0^2 - 4c_2^2 - c_4^2 \ge 10a_0^2 - 8a_0^2 - 2a_0^2 = 0. \tag{39}$$

All in all, the positive semi-definiteness of the fourth order orientation tensor yields the condition

$$0 \le 2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2 \tag{40}$$

for the Fourier coefficients a_0, a_2, a_4, b_2, b_4. This condition can be extended to coefficients of higher order with a more general orientation tensor $\mathbb{B}_4^{(m)}$ as in the case of $\mathbb{B}_2^{(m)}$ (see equation (34))

$$0 \le 2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_m^2 - \sqrt{2}a_0c_{2m}^2 + 2a_m^2a_{2m} + 4a_mb_mb_{2m} - 2a_{2m}b_m^2. \tag{41}$$

Furthermore it is possible to define irregular tensors like

$$
\begin{aligned}
\widehat{\mathbb{B}} &= \int_0^{2\pi} \begin{pmatrix} \cos(3\phi)\cos(3\phi) & \cos(3\phi)\sin(\phi) \\ \sin(\phi)\cos(3\phi) & \sin(\phi)\sin(\phi) \end{pmatrix} \psi(\phi)\,\mathrm{d}\phi \\
&= \frac{1}{2}\int_0^{2\pi} \begin{pmatrix} 1+\cos(6\phi) & \sin(4\phi)-\sin(2\phi) \\ \sin(4\phi)-\sin(2\phi) & 1-\cos(2\phi) \end{pmatrix} \psi(\phi)\,\mathrm{d}\phi \qquad (42) \\
&= \frac{\sqrt{\pi}}{2} \begin{pmatrix} \sqrt{2}a_0 + a_6 & b_4 - b_2 \\ b_4 - b_2 & \sqrt{2}a_0 - a_2 \end{pmatrix},
\end{aligned}
$$

which also satisfy the condition of positive semi-definiteness of theorem 4.3. Then the characteristic polynomial of $\widehat{\mathbb{B}}$ is given by

$$
\begin{aligned}
\chi_{\widehat{\mathbb{B}}}(\lambda) &= \det(\lambda \boldsymbol{\mathcal{I}} - \widehat{\mathbb{B}}) = \det(\sqrt{\pi}\tilde{\lambda}\boldsymbol{\mathcal{I}} - \widehat{\mathbb{B}}) \\
&= \tfrac{\pi}{4}\left[(2\tilde{\lambda} - \sqrt{2}a_0 - a_6)(2\tilde{\lambda} - \sqrt{2}a_0 + a_2) - (b_4 - b_2)^2\right] \\
&= \tfrac{\pi}{4}\Big[4\tilde{\lambda}^2 - (4\sqrt{2}a_0 - 2a_2 + 2a_6)\tilde{\lambda} \qquad (43) \\
&\qquad + 2a_0^2 - \sqrt{2}a_0a_2 + \sqrt{2}a_0a_6 - a_2a_6 - (b_4 - b_2)^2\Big].
\end{aligned}
$$

where $\tilde{\lambda} = \frac{\lambda}{\sqrt{\pi}}$, and the conditions

$$
\begin{cases}
0 \leq 2\sqrt{2}a_0 - a_2 + a_6, & \text{(44a)} \\
0 \leq 2a_0^2 - \sqrt{2}a_0a_2 + \sqrt{2}a_0a_6 - a_2a_6 - (b_4 - b_2)^2, & \text{(44b)}
\end{cases}
$$

must be valid, where the first one is true due to inequalities (36b).

5. Correction techniques

In the last section, we have analyzed the properties of orientation tensors associated with a nonnegative Fourier approximation $\psi^{N_{\mathbf{p}}}$ and derived corresponding conditions for the Fourier coefficients. While it is nearly impossible to take all possible inequalities for a "nonnegative" Fourier approximation $\psi^{N_{\mathbf{p}}}$ of high order $N_{\mathbf{p}} \gg 2$ into account, we are now able to verify if specific orientation tensors, like the ones appearing in the definition of the effective stress tensor τ_{eff} (see equation (9)), are positive semi-definite and therefore physics-compatible without solving an eigenvalue problem each time. This section deals with two methods which correct the coefficients of $\psi^{N_{\mathbf{p}}}$ if the corresponding (known) relations are not satisfied.

After discretizing the space-independent Fokker-Planck equation (18) in the orientation component as described in section 3 and using the θ-method for the time discretization, we obtain the linear system

$$\boldsymbol{\mathcal{A}}\boldsymbol{\psi}^{n+1} := \left(\boldsymbol{\mathcal{M}} + \Delta t\theta(\boldsymbol{\mathcal{K}} + \boldsymbol{\mathcal{D}})\right)\boldsymbol{\psi}^{n+1} = \left(\boldsymbol{\mathcal{M}} - \Delta t(1-\theta)(\boldsymbol{\mathcal{K}} + \boldsymbol{\mathcal{D}})\right)\boldsymbol{\psi}^{n} =: \mathbf{b}, \tag{45}$$

where $\boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{M}}, \boldsymbol{\mathcal{K}}, \boldsymbol{\mathcal{D}} \in \mathbb{R}^{N_\mathbf{p}+1\times N_\mathbf{p}+1}$ are the system, mass, convection and diffusion matrices, respectively, and

$$\boldsymbol{\psi}^n = \left(a_0^n, b_2^n, a_2^n, \dots, b_{N_\mathbf{p}}^n, a_{N_\mathbf{p}}^n\right)^\top = \left(\psi_0^n, \psi_1^n, \dots, \psi_{N_\mathbf{p}}^n\right)^\top \quad \in \quad \mathbb{R}^{N_\mathbf{p}+1} \tag{46}$$

defines the vector of Fourier coefficients of the approximation $\psi^{N_\mathbf{p}}$ at the time level $t = t^n$, i.e., $\psi^{N_\mathbf{p},n} = \psi^{N_\mathbf{p}}(t^n) \approx \psi(t^n)$. In general, the solution $\psi^{N_\mathbf{p}}$ defined by the coefficients $\boldsymbol{\psi}^{n+1} = \boldsymbol{\mathcal{A}}^{-1}\mathbf{b}$ does not ensure nonnegativity or the conditions deduced in section 4. To enforce these conditions, we correct the coefficients by solving the constrained least-squares problem

$$\begin{cases} F(\boldsymbol{\psi}^{n+1}) = \left\|\boldsymbol{\mathcal{P}}^{-1}(\boldsymbol{\mathcal{A}}\boldsymbol{\psi}^{n+1} - \mathbf{b})\right\|_2^2 \quad = \quad \min!, & \text{(47a)} \\ \quad c_{2k}^{n+1} \leq \sqrt{2}a_0^{n+1} \qquad\qquad \text{for all } 1 \leq k \leq N_\mathbf{p}, & \text{(47b)} \\ \quad 0 \leq 2\sqrt{2}(a_0^{n+1})^3 - 2\sqrt{2}a_0^{n+1}(c_2^{n+1})^2 - \sqrt{2}a_0^{n+1}(c_4^{n+1})^2 \\ \qquad + 2(a_2^{n+1})^2 a_4^{n+1} + 4a_2^{n+1}b_2^{n+1}b_4^{n+1} - 2a_4^{n+1}(b_2^{n+1})^2, & \text{(47c)} \\ \quad a_0^{n+1} = a_0^n, & \text{(47d)} \end{cases}$$

where equations (47b) and (47c) define the range of admissible values for the Fourier coefficients of $\boldsymbol{\psi}^{n+1}$, inequality (47d) ensures mass conservation and $\boldsymbol{\mathcal{P}}^{-1} \in \mathbb{R}^{N_\mathbf{p}+1\times N_\mathbf{p}+1}$ stands for a suitable preconditioner. By choosing $\boldsymbol{\mathcal{P}}^{-1} = \boldsymbol{\mathcal{I}}$, the error norm of the residual $\boldsymbol{\mathcal{A}}\boldsymbol{\psi}^{n+1} - \mathbf{b}$ would be minimized under the above-mentioned conditions. If we define $\boldsymbol{\mathcal{P}}^{-1} = \boldsymbol{\mathcal{A}}^{-1}$, the distance to an unphysical approximation $\tilde{\psi}^{N_\mathbf{p}}(t^{n+1})$ with the coefficient vector $\tilde{\boldsymbol{\psi}}^{n+1} = \boldsymbol{\mathcal{A}}^{-1}\mathbf{b}$ would be reduced. This choice is justifiable due to the equality

$$\|\boldsymbol{\psi}^{n+1} - \tilde{\boldsymbol{\psi}}^{n+1}\|_2^2 = \int_0^{2\pi} \left(\psi^{N_\mathbf{p}}(\phi, t^{n+1}) - \tilde{\psi}^{N_\mathbf{p}}(\phi, t^{n+1})\right)^2 \mathrm{d}\phi \tag{48}$$

and is used in the following.

If condition (47c) for a positive semi-definite fourth order orientation tensor $\mathbb{A}_4$ is neglected, the minimization problem (47) decomposes into local subproblems which can be analyzed independently. After solving these subproblems analytically, the Fourier coefficients of $\psi^{N_{\mathbf{p}}}(t^{n+1})$ are defined by [13]

$$
\begin{aligned}
a_k &= \sqrt{2}a_0^{n+1}\tilde{(}c_k^{n+1})^{-1}\tilde{a}_k^{n+1} = \gamma_k^{n+1}\tilde{a}_k^{n+1}, \\
b_k &= \sqrt{2}a_0^{n+1}\tilde{(}c_k^{n+1})^{-1}\tilde{b}_k^{n+1} = \gamma_k^{n+1}\tilde{b}_k^{n+1},
\end{aligned}
\tag{49}
$$

where $\gamma_k^{n+1} = \sqrt{2}a_0^{n+1}(\tilde{c}_k^{n+1})^{-1}$. If we wish to ensure the positive semi-definiteness of $\mathbb{A}_4$, too, $b_2^{n+1}, a_2^{n+1}, b_4^{n+1}$ and a_4^{n+1} have to satisfy the reduced minimization problem

$$
\begin{cases}
F(\ldots) = \displaystyle\sum_{k=1}^{2}(a_{2k}^{n+1} + \tilde{a}_{2k}^{n+1})^2 + (b_{2k}^{n+1} + \tilde{b}_{2k}^{n+1})^2 \quad = \quad \min!, & \text{(50a)} \\
c_2^{n+1} \leq \sqrt{2}a_0^{n+1} & \text{(50b)} \\
c_4^{n+1} \leq \sqrt{2}a_0^{n+1} & \text{(50c)} \\
\quad 0 \leq 2\sqrt{2}(a_0^{n+1})^3 - 2\sqrt{2}a_0^{n+1}(c_2^{n+1})^2 - \sqrt{2}a_0^{n+1}(c_4^{n+1})^2 & \\
\qquad + 2(a_2^{n+1})^2 a_4^{n+1} + 4a_2^{n+1}b_2^{n+1}b_4^{n+1} - 2a_4^{n+1}(b_2^{n+1})^2, & \text{(50d)}
\end{cases}
$$

and the additional coefficients a_k^{n+1} and b_k^{n+1} for $k > 4$ can be defined by equation (49).

Another approach to enforcing the conditions of positive semi-definiteness is based on stabilization techniques for Galerkin discretizations of pure convection equations: artificial diffusion is added to dampen possible (especially high-frequency) oscillations. This can guarantee nonnegativity because the constant orientation distribution function $\psi^{N_{\mathbf{p}}} \equiv \text{const}$ satisfies the nonnegativity condition $\psi^{N_{\mathbf{p}}} \geq 0$ in all cases. To utilize the artificial diffusion approach and define the artificial diffusion parameter $\tilde{\mu} \geq 0$, we apply another operator splitting to the modified partial differential equation

$$
\frac{\partial \psi(\mathbf{p}, t)}{\partial t} + \operatorname{div}_{\mathbf{p}}\left(\dot{\mathbf{p}}\psi(\mathbf{p}, t)\right) - \Delta_{\mathbf{p}}\left(D_r \psi(\mathbf{p}, t)\right) - \tilde{\mu}\Delta_{\mathbf{p}}\left(\psi(\mathbf{p}, t)\right) = 0. \tag{51}
$$

The resulting additional initial value problem reads

$$
\frac{\partial \psi}{\partial t} - \tilde{\mu}\Delta_{\mathbf{p}}\left(\psi(\mathbf{p}, t)\right) = 0 \qquad \text{in } (t^n, t^{n+1}) \qquad \text{with} \qquad \psi(t^n) = \tilde{\psi}^{n+1} \tag{52}
$$

and the corresponding discrete problem is given by

$$
\boldsymbol{\mathcal{A}}_{\tilde{\boldsymbol{\mathcal{D}}}}\boldsymbol{\psi}^{n+1} := \left(\boldsymbol{\mathcal{M}} + \mu\theta\tilde{\boldsymbol{\mathcal{D}}}\right)\boldsymbol{\psi}^{n+1} = \left(\boldsymbol{\mathcal{M}} - \mu(1-\theta)\tilde{\boldsymbol{\mathcal{D}}}\right)\tilde{\boldsymbol{\psi}}^{n+1} =: \mathbf{b}_{\tilde{\boldsymbol{\mathcal{D}}}}, \tag{53}
$$

where $\mu := \Delta t\tilde{\mu}$. The minimization problem for calculating $\mu \geq 0$ reads

$$
\begin{cases}
F(\mu) = \mu \quad = \quad \min!, & (54a)\\
c_{2k}^{n+1} \leq \sqrt{2}a_0^{n+1} \qquad\qquad \text{for all } 1 \leq k \leq N_{\mathbf{p}}, & (54b)\\
\quad 0 \leq 2\sqrt{2}(a_0^{n+1})^3 - 2\sqrt{2}a_0^{n+1}(c_2^{n+1})^2 - \sqrt{2}a_0^{n+1}(c_4^{n+1})^2 & \\
\qquad + 2(a_2^{n+1})^2 a_4^{n+1} + 4a_2^{n+1}b_2^{n+1}b_4^{n+1} - 2a_4^{n+1}(b_2^{n+1})^2, & (54c)\\
a_0^{n+1} = \tilde{a}_0^{n+1}, & (54d)
\end{cases}
$$

with a_k^{n+1} and b_k^{n+1} defined by [13]

$$
a_k^{n+1} = \frac{\pi - k^2\pi\mu(1-\theta)}{\pi + k^2\pi\mu\theta}\tilde{a}_k^{n+1} = \big(1 - \frac{k^2\mu}{1 + k^2\mu\theta}\big)\tilde{a}_k^{n+1}, \tag{55a}
$$

$$
b_k^{n+1} = \frac{\pi - k^2\pi\mu(1-\theta)}{\pi + k^2\pi\mu\theta}\tilde{b}_k^{n+1} = \big(1 - \frac{k^2\mu}{1 + k^2\mu\theta}\big)\tilde{b}_k^{n+1} \tag{55b}
$$

because of the diagonal form of the mass and diffusion matrices $\boldsymbol{\mathcal{M}}$ and $\tilde{\boldsymbol{\mathcal{D}}}$, respectively. Here we have to observe the condition

$$
1 \geq \frac{k^2\mu}{1 + k^2\mu\theta} \qquad \Rightarrow \qquad 1 - \tfrac{1}{k^2\mu} \leq \theta \leq 1 \qquad \text{for all } 1 \leq k \leq N_{\mathbf{p}}, \tag{56}
$$

because a change in sign of the coefficients a_k^{n+1} and b_k^{n+1} is unphysical after adding pure diffusion. Problem (55) decomposes into local subproblems as well, where the decomposition depends on the inequalities. Then μ must be defined as the minimum of artificial diffusion parameters for all subproblems. If we only take care of conditions (54b) and (54d) and ignore the positive semi-definiteness of the fourth order tensor $\mathbb{A}_4$ (inequality (54c)), then $\mu \geq 0$ has to satisfy [13]

$$
\mu = \max\Big\{0, \frac{\tilde{c}_k^{n+1} - \sqrt{2}a_0}{k^2(\theta\sqrt{2}a_0 + (1-\theta)\tilde{c}_k^{n+1})}\Big\} \qquad \text{for all } 1 \leq k \leq N_{\mathbf{p}}. \tag{57}
$$

A detailed derivation of the results of equations (49), (55), and (57) is presented in [13].

6. Generalization to 3D

After analyzing nonnegative Fourier approximations of planar orientation distribution functions $\psi : \mathbb{S}^1 \to \mathbb{R}_0^+$ and designing correction techniques for the Fourier coefficients, let us now summarize the equivalent results for more general three-dimensional orientation distribution functions $\psi : \mathbb{S}^2 \to \mathbb{R}_0^+$ using spherical coordinates defined by $\mathbf{p}(\theta, \phi) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^\top$ with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$. For this problem, the corresponding basis functions of the Galerkin discretization are given by the real-valued spherical harmonics $Y_{l,m}$ with $2l \in \mathbb{N}_0$ and $-l \leq m \leq l$, which are defined by

$$Y_{l,m} = \begin{cases} \sqrt{2}(-1)^m \mathrm{Im}(Y_l^{|m|}) & : m < 0, \\ Y_l^0 & : m = 0, \\ \sqrt{2}(-1)^m \mathrm{Re}(Y_l^{|m|}) & : m > 0. \end{cases} \tag{58}$$

The complex spherical harmonics Y_l^m form a complete and orthonormal set of eigenfunctions of the Laplace-Beltrami operator defined on the two-dimensional sphere

$$\Delta_{\theta,\phi} Y_l^m(\theta, \phi) = \big(\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\big) Y_l^m(\theta, \phi) \tag{59}$$

$$= -l(l+1) Y_l^m(\theta, \phi) \tag{60}$$

and are given by

$$Y_l^m(\theta, \phi) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}} P_{l,m}(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi}, \tag{61}$$

where $P_{l,m}$ are the associated Legendre polynomials and $l \in \mathbb{N}_0,\ -l \leq m \leq l$. We just need to consider $Y_{l,m}$ with l even because the parity only depends on the index l. In particular, $Y_l^m(\pi - \theta, \pi + \phi) = (-1)^l Y_l^m(\theta, \phi)$. Additionally, l determines the order of $Y_{l,m}$, so the number of basis functions with an order less than or equal to $N_\mathbf{p}$ is given by $(\frac{N_\mathbf{p}}{2} + 1)(N_\mathbf{p} + 1)$.

As in the planar case considered in section 4, all square integrable (real-valued) functions $\psi : \mathbb{S}^2 \to \mathbb{R}$ (with an even parity) can be represented by a series of spherical harmonics in spherical coordinates

$$\psi(\theta, \phi) = \sum_{l \in \mathbb{N}_0} \sum_{-l \leq m \leq l} \psi_{2l,m} Y_{2l,m}(\theta, \phi). \tag{62}$$

Therefore, an approximation of order $N_\mathbf{p}$ is given by the truncated series

$$\psi^{N_\mathbf{p}}(\theta, \phi) = \sum_{l=0}^{N_\mathbf{p}} \sum_{m=-l}^{l} \psi_{2l,m} Y_{2l,m}(\theta, \phi) \quad \approx \quad \psi(\theta, \phi), \tag{63}$$

where the "mass" is given by the coefficient $\psi_{0,0}$ and should again satisfy the normalization condition (1) or (12).

Theorems like the one on positive semi-definiteness of a tensor (theorem 4.3) and Descartes' rule of signs (theorem 4.2) are defined generically. Therefore, we can adopt them for three-dimensional orientation distribution functions ψ and derive inequalities for their nonnegativity, too. For example, after expressing $\mathbf{p}_i\mathbf{p}_j$ in terms of the real-valued spherical harmonics $Y_{0,0}, Y_{2,-2}, \ldots, Y_{2,2}$, the second order orientation tensor $\mathbb{A}_2 \in \mathbb{R}^{3\times 3}$ reads

$$\mathbb{A}_2 = \frac{2\sqrt{\pi}}{3\sqrt{15}} \begin{pmatrix} c_1 & 3\psi_{2,-2} & 3\psi_{2,1} \\ 2\psi_{2,-2} & c_2 & 3\psi_{2,-1} \\ 3\psi_{2,1} & 3\psi_{2,-1} & c_3 \end{pmatrix}, \tag{64}$$

where $c_1, c_2, c_3 \in \mathbb{R}$ are defined by

$$c_1 = 3\psi_{2,2} - \sqrt{3}\psi_{2,0} + \sqrt{15}a_0^0, \tag{65a}$$

$$c_2 = -3\psi_{2,2} - \sqrt{3}\psi_{2,0} + \sqrt{15}a_0^0, \tag{65b}$$

$$c_3 = 2\sqrt{3}\psi_{2,0} + \sqrt{15}a_0^0. \tag{65c}$$

Then the characteristic polynomial $\chi_{\mathbb{A}_2}$ yields the conditions

$$\begin{cases} 0 \leq \psi_{0,0}, & (66a) \\ 0 \leq 5\psi_{0,0}^2 - \psi_{2,-2}^2 - \psi_{2,-1}^2 - \psi_{2,0}^2 - \psi_{2,1}^2 - \psi_{2,2}^2, & (66b) \\ 0 \leq 15\sqrt{15}\psi_{0,0}^3 + 27\psi_{2,2}\left(\psi_{2,1}^2 - \psi_{2,-1}^2\right) + 54\psi_{2,-2}\psi_{2,-1}\psi_{2,1} & \\ \quad - 3\sqrt{3}\psi_{2,0}\left(6\psi_{2,-2}^2 - 3\psi_{2,-1}^2 - 2\psi_{2,0}^2 - 3\psi_{2,1}^2 + 6\psi_{2,2}^2\right) & (66c) \\ \quad - 9\sqrt{15}\psi_{0,0}\left(\psi_{2,-2}^2 + \psi_{2,-1}^2 + \psi_{2,0}^2 + \psi_{2,1}^2 + \psi_{2,2}^2\right). & \end{cases}$$

Similarly, it is possible to derive conditions for other coefficients by analyzing the associated tensors but inequalities corresponding to tensors of higher orders become more and more complicated and their derivation is left to the reader. Spherical harmonics approximations preserving the positive semi-definiteness of orientation tensors can be constructed using straightforward extensions of the correction methods introduced in section 5.

7. Numerical examples

To validate the correction procedures for nonnegative orientation distribution functions, we focus on planar test cases with a constant velocity

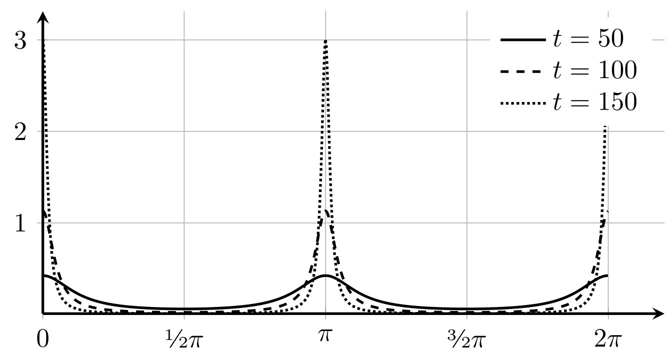

Figure 2: Analytical solution of the planar elongational flow at different points of time.

gradient and no diffusion, i.e., $C_I = 0$. Altan and Tang [4] presented analytical solutions for such configurations with random initial distributions, i.e., $\psi(\cdot, t = 0) = \text{const}$. To study the effect of the proposed corrections on approximate solutions of the Fokker-Planck equation, let us focus on the "planar elongational flow" with the velocity gradient defined by

$$\nabla_{\mathbf{x}} \mathbf{u} = \begin{pmatrix} 0.01 & 0 \\ 0 & -0.01 \end{pmatrix} \in \mathbb{R}^{2\times 2} \tag{67}$$

and an aspect ratio of the fibers of $r_e = 10$ (for example length $L = 1\,\text{mm}$ and diameter $d = 0.1\,\text{mm}$), i.e., $\lambda = \frac{99}{101}$. This problem is deformation dominant with the preferred orientation $\mathbf{p}^* = (1, 0)^\top$ of the fibers. Figure 2 shows the corresponding analytical solution at different time instants.

The space-independent Fokker-Planck equation (18) is discretized using a Fourier approximation of order $N_{\mathbf{p}} = 6$ and the Crank-Nicolson method ($\theta = \frac{1}{2}$) for discretization in time with the time step $\Delta t = 1$. The following figures illustrate the performance of the correction methods "Minimization" (Min.) and "Diffusion" (Diff.) in comparison to the uncorrected Galerkin method and the analytical solution. In the process of correction, the coefficient c_k is adjusted and, additionally, the positive semi-definiteness of $\mathbb{A}_4$ is enforced. As expected, the correction methods preserve positive semi-definiteness of the orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$, if configured to do so (see figures 3 and 4). The results for the two versions differ in the restriction of high-frequency oscillations (see figure 5). The artificial diffusion approach damps high-frequency oscillations more intensively. A further side benefit of correcting the coefficients is the reduction of the Euclidean error norm of

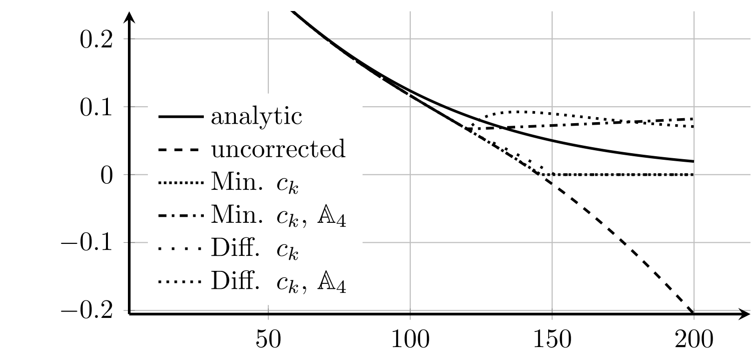

Figure 3: Minimal eigenvalue of the second order orientation tensor $\mathbb{A}_2$ of the planar elongational flow with a Fourier approximation of order $N_{\mathbf{p}} = 6$ depending on the time.

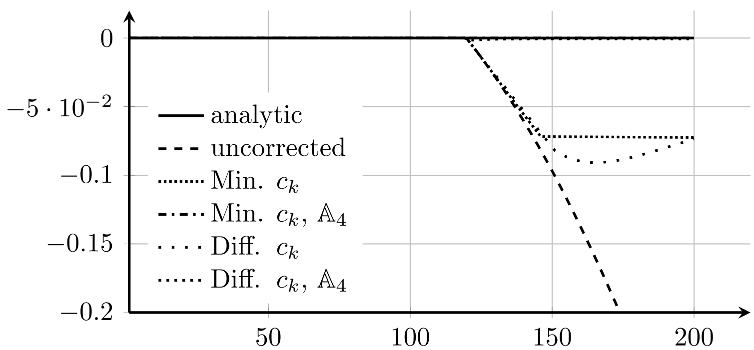

Figure 4: Minimal eigenvalue of the fourth order orientation tensor $\mathbb{A}_4$ of the planar elongational flow with a Fourier approximation of order $N_{\mathbf{p}} = 6$ depending on the time.

the first Fourier coefficients (see figure 6), which is likely to produce more accurate orientation tensors $\mathbb{A}_2$ and $\mathbb{A}_4$ (see figures 7 and 8, respectively).

8. Conclusions and outlook

In this paper, we developed correction methods for Fourier approximations of nonnegative orientation distribution functions. For this purpose, a weak definition of nonnegativity was introduced. The proposed criterion allows small undershoots and thereby exact truncated series expansions of nonnegative functions. For such approximations, inequalities for the Fourier coefficients could be established on the basis of positive semi-definite orientation tensors. The corresponding conditions make it possible to verify positive semi-definiteness without evaluating the function at a considerable number of

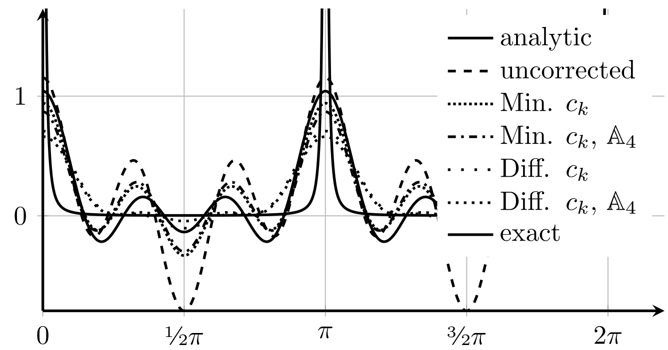

Figure 5: Final approximation $\psi^{N_\mathbf{p}}$ at $t = 200$ of the planar elongational flow with a Fourier approximation of order $N_\mathbf{p} = 6$.

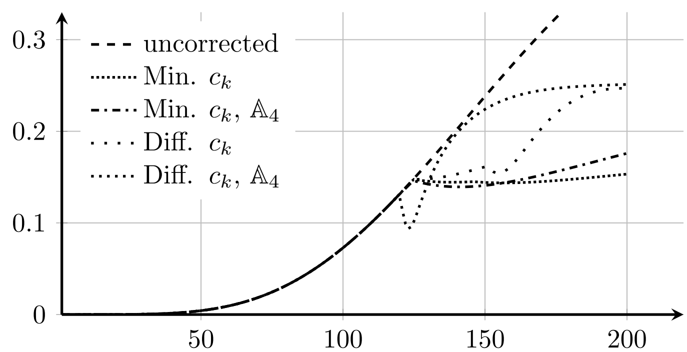

Figure 6: Euclidean error norm of the first Fourier coefficients of the planar elongational flow with a Fourier approximation of order $N_\mathbf{p} = 6$ depending on the time.

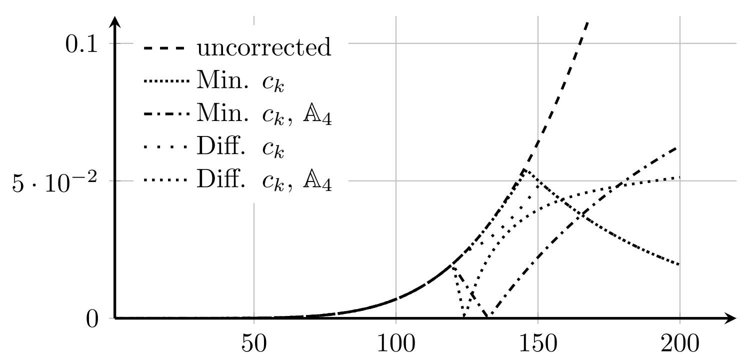

Figure 7: Euclidean error norm of the second order orientation tensor $\mathbb{A}_2$ of the planar elongational flow with a Fourier approximation of order $N_\mathbf{p} = 6$ depending on the time.

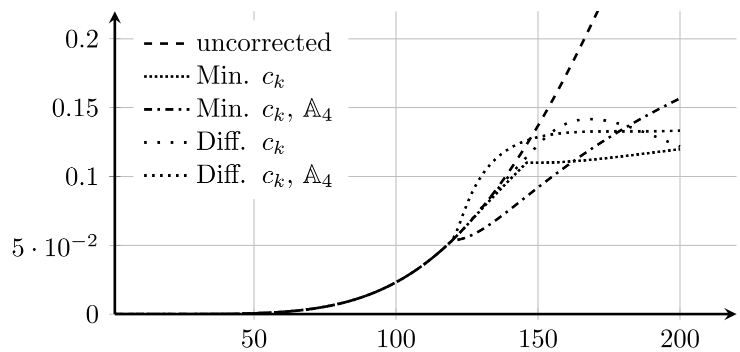

Figure 8: Euclidean error norm of the fourth order orientation tensor $\mathbb{A}_4$ of the planar elongational flow with a Fourier approximation of order $N_{\mathbf{p}} = 6$ depending on the time.

points. Also, we have introduced correction techniques which guarantee weak nonnegativity by solving minimization problems with nonlinear constraints. These corrections significantly reduce spurious oscillations by enforcing inequality conditions that are known to hold for a nonnegative function with the first Fourier coefficients equal to those of the approximate solution.

The disadvantages of this fast approach to constraining the Fourier coefficients are the complexity of inequalities which are associated with tensors of high order and the uncertainty regarding the completeness of the nonnegativity conditions. Thus the proposed strategy is feasible only for Fourier approximations of low order (e.g., $N_{\mathbf{p}} = 2, 4$) for which a verification of such conditions is practically achievable. In a forthcoming paper, we will present an alternative method which enforces nonnegativity conditions for Fourier approximations of arbitrary order without imposing inequality constraints on the coefficients. In this method, our definition of nonnegativity for Fourier approximations is satisfied by designing a nonnegative function ψ with $\mathcal{P}_{N_{\mathbf{p}}}\psi = \psi^{N_{\mathbf{p}}}$ making use of exponential reconstructions.

As mentioned in section 6, all concepts and and algorithms developed in the context of Fourier approximations carry over to the more general three-dimensional case, in which the orthonormal Fourier basis functions are replaced by real-valued spherical harmonics. It is hoped that the proposed correction methods will contribute to obtaining more realistic solutions of the Fokker-Planck equation (11) when it comes to physics-compatible simulations of fiber suspensions on the basis of the generalized Navier-Stokes equations.

Acknowledgements

This research was supported by the German Research Association (DFG) under grant KU 1530/13-1.

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